

LASER SPECTROSCOPY OF THE $A^2\Pi - X^2\Sigma^+$ TRANSITION OF YTTERBIUM MONOACETYLIDE

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The first spectroscopic identification and characterization of ytterbium monoacetylide (YbCCH) and two of its isotopomers is reported. By combining resonance enhanced two photon ionization (R2PI), laser induced fluorescence (LIF), and photoionization efficiency spectroscopy (PIE) with density functional calculations the $X^2\Sigma^+$ and the $A^2\Pi_{1/2,3/2}$ states of YbCCH and the $X^1\Sigma^+$ state of YbCCH⁺ have been characterized.

The $A^2\Pi - X^2\Sigma^+$ system whose 0-0 band for the $A^2\Pi_{1/2}$ component lies at around 16848 cm⁻¹ for YbCCH ($A_{SO} = 1411$ cm⁻¹) has been studied at 0.3 cm⁻¹ resolution. The excitation spectra, both R2PI and fluorescence, are characterized by progressions and sequences involving the YbCC bending mode, ν_5 , whose wavenumber has been determined to be 93 cm⁻¹ and 103 cm⁻¹ for the $X^2\Sigma^+$ and the $A^2\Pi_{1/2,3/2}$ state, respectively. The dispersed fluorescence spectra show a progression in the ground state YbC stretching mode with a wavenumber of $\omega(\nu_3) = 328$ cm⁻¹.

Density functional calculations confirmed the vibrational assignment and yielded a linear geometry for both the X - and A - state of YbCCH as well as for the $X^1\Sigma^+$ state of the cation.

Photoionization efficiency spectroscopy yielded an adiabatic ionization potential of 47165(10) cm⁻¹ (5.8477 eV). Rydberg series converging to the $v^+ = 1$ and $v^+ = 2$ level of YbCCH⁺ were observed and combined with the ion-appearance potentials led to $\omega(\nu_5) = 97$ cm⁻¹ for the YbCC bending mode in YbCCH⁺.

A high resolution study of the $A^2\Pi - X^2\Sigma^+$ system of YbCCH is currently in progress and results may be available at the time of the meeting.